

Vortex lattice structures and pairing symmetry in Sr_2RuO_4

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Recent experimental results indicate that superconductivity in Sr_2RuO_4 is described by the p -wave E_u representation of the D_{4h} point group. Results on the vortex lattice structures for this representation are presented. The theoretical results are compared with experiment.

1. Introduction

The oxide Sr_2RuO_4 has a structure similar to high T_c materials and was observed to be superconducting by Maeno *et al.* in 1994 [1]. It has been established that this superconductor is not a conventional s -wave superconductor: NQR measurements show no indication of a Hebel-Slichter peak in $1/T_1T$ [2], and T_c is strongly suppressed below the maximum value of 1.5 K by non-magnetic impurities [3]. More recent experiments indicate an odd parity gap function of the form $\mathbf{d}(\mathbf{k}) = \hat{z}(\eta_x k_x + \eta_y k_y)$. The Knight shift measurements of Ishida *et al.* [4] reveal that the spin susceptibility is unchanged upon entering the superconducting state; this is consistent with p -wave superconductivity (as predicted by Rice and Sigrist [5]). Furthermore, these measurements were conducted with the applied field in the basal plane. Since the orientation of the gap function (that is \mathbf{d}) is orthogonal to the spin projection of the Cooper pair [6], these measurements are consistent with the gap function aligned along the \hat{z} direction. The μSR experi-

ments of Luke *et al.* have revealed spontaneous fields in the Meissner state [7]. This indicates that the superconducting order parameter must have more than one component [6,7]. Naively, the observation of spontaneous fields leads to the conclusion that the superconducting gap function breaks time reversal symmetry (\mathcal{T}) and therefore must have the form $\mathbf{d}(\mathbf{k}) = \hat{z}(k_x \pm ik_y)$. However, the muons probe inhomogeneities in the superconducting state since any bulk magnetic fields are screened in the Meissner state. Consequently, \mathcal{T} need only be broken in the vicinity of the inhomogeneities. For example, it has been pointed out in Ref. [6] that a gap function given by $\vec{\eta} = (1, \pm 1)$ can give rise to domain walls that break time reversal symmetry. In principle this can also lead to a μSR signal as seen by Luke *et al.*. Consequently, these two experiments lead to the gap function $\mathbf{d}(\mathbf{k}) = \hat{z}(\eta_x k_x + \eta_y k_y)$, with the specific form of the order parameter η_x and η_y undetermined. In this talk, the vortex lattice structures arising in the phenomenological theory of this E_u representation are examined. First, the theory is examined for an applied magnetic field in the

basal plane along one of the two-fold symmetry axes. It is shown that multiple vortex lattice phases are generic to this representation. Then the weak-coupling limit of the theory is examined for the applied magnetic field along the c -axis. It is shown that a square vortex lattice results for parameters relevant to Sr_2RuO_4 ; consistent with the experimental observation of a square vortex lattice [8]. The theory of the square vortex lattice is compared with the observed results and good agreement is found.

2. Free Energy

The dimensionless free energy for the E_u representation of D_{4h} is given by [6]

$$\begin{aligned} f = & -|\vec{\eta}|^2 + |\vec{\eta}|^4/2 + \beta_2(\eta_x\eta_y^* - \eta_y\eta_x^*)^2/2 \\ & + \beta_3|\eta_x|^2|\eta_y|^2 + |\tilde{D}_x\eta_x|^2 + |\tilde{D}_y\eta_y|^2 \\ & + \kappa_2(|\tilde{D}_y\eta_x|^2 + |\tilde{D}_x\eta_y|^2) \\ & + \kappa_5(|\tilde{D}_z\eta_x|^2 + |\tilde{D}_z\eta_y|^2) \\ & + \kappa_3[(\tilde{D}_x\eta_x)(\tilde{D}_y\eta_y)^* + h.c.] \\ & + \kappa_4[(\tilde{D}_y\eta_x)(\tilde{D}_x\eta_y)^* + h.c.] + h^2/(8\pi). \end{aligned} \quad (1)$$

where $\tilde{D}_j = \nabla_j - \frac{2ie}{\hbar c}A_j$, $\mathbf{h} = \nabla \times \mathbf{A}$, and \mathbf{A} is the vector potential. The stable homogeneous solutions are easily determined. There are three phases: (a) $\vec{\eta} = (1, i)/\sqrt{2}$ ($\beta_2 > 0$ and $\beta_2 > \beta_3/2$), (b) $\vec{\eta} = (1, 0)$ ($\beta_3 > 0$ and $\beta_2 < \beta_3/2$), and (c) $\vec{\eta} = (1, 1)/\sqrt{2}$ ($\beta_3 < 0$ and $\beta_2 < 0$). Phase (a) is nodeless and phases (b) and (c) have line nodes. For some of the discussion in this paper the Ginzburg Landau coefficients are determined within a weak-coupling approximation in the clean limit. In this case, taking for the E_u REP the gap function described by the pseudo-spin-pairing gap matrix: $\hat{\Delta} = i[\eta_1 v_x/\sqrt{\langle v_x^2 \rangle} + \eta_2 v_y/\sqrt{\langle v_y^2 \rangle}]\sigma_z\sigma_y$, where the brackets $\langle \rangle$ denote an average over the Fermi surface and σ_i are the Pauli matrices, it is found that [9] $\beta_2 = \kappa_2 = \kappa_3 = \kappa_4 = (\nu + 1)/(3 - \nu)$ and $\beta_3 = 4\nu/(3 - \nu)$ where

$$\nu = \frac{\langle v_x^4 \rangle - 3\langle v_x^2 v_y^2 \rangle}{\langle v_x^4 \rangle + \langle v_x^2 v_y^2 \rangle}. \quad (2)$$

Note that $|\nu| \leq 1$ and $\nu = 0$ for a spherical or a cylindrical Fermi surface. Also note that $\vec{\eta} \propto (1, i)$ is the stable homogeneous state for all ν .

3. Magnetic field in the basal plane

For the E_u model, symmetry arguments imply that the vortex lattice phase diagram contains at least two vortex lattice phases for magnetic fields applied along at least two of the four two-fold symmetry axes [9]. To demonstrate this, consider the magnetic field along the \hat{x} direction (\hat{x} is chosen to be along the crystal \mathbf{a} axis) and a homogeneous zero-field state $\vec{\eta} \propto (1, i)$. The presence of a magnetic field along the \hat{x} direction breaks the degeneracy of the (η_x, η_y) components, so that only one of these two components will order at the upper critical field [*e.g.* $\vec{\eta} \propto (0, 1)$]. It has been shown for type II superconductors with a single component order parameter that the solution is independent of x [10] so that σ_x (a reflection about the \hat{x} direction) is a symmetry operation of the $\vec{\eta} \propto (0, 1)$ vortex phase. Now consider the zero-field phase $\vec{\eta} \propto (1, i)$; σ_x transforms $(1, i)$ to $(-1, i) \neq e^{i\psi}(1, i)$ where ψ is phase factor. This implies that σ_x is *not* a symmetry operator of the zero-field phase. It follows that there must exist a second transition in the finite field phase at which η_x becomes non-zero. Similar arguments hold for the field along any of the other three two-fold symmetry directions in the basal plane. Consequently a zero-field state $\vec{\eta} \propto (1, i)$ must exhibit two vortex lattice phases when the field is applied along any of the four two-fold symmetry axes. Similar arguments for $\vec{\eta} \propto (1, 0)$ or $\vec{\eta} \propto (1, 1)$ imply that there must exist at least two vortex lattice phases for only two of the four two-fold symmetry axes. For a zero-field state $\vec{\eta} = (1, 0)$ fields along the $(1, 1)$ or the $(1, -1)$ directions will result in two vortex lattice phases (for the $(1, 0)$ and the $(0, 1)$ directions multiple vortex lattice phases may exist, but are not required by symmetry). For a zero-field state $\vec{\eta} \propto (1, 1)$, two vortex lattice phases will exist for fields along the $(1, 0)$ or the $(0, 1)$ directions.

An analysis of the free energy of Eq. 1 reveals additional information about the phase diagram [9,11]. Assuming the large κ limit (note $\kappa \approx 30$ for this field orientation in Sr_2RuO_4), the vector potential can be taken to be $\mathbf{A} = H z(\sin \phi, -\cos \phi, 0)$ (ϕ is the angle in the basal plane that the applied magnetic field makes with

the \hat{x} direction). The component of \mathbf{D} along the field is set to zero. The upper critical field found by this method exhibits a four-fold anisotropy in the basal plane [9,6]. For concreteness, the field is taken along the \hat{x} direction ($\phi = 0$). Introducing the raising and lowering operators $\Pi_{\pm} = q(\sqrt{\kappa_2/\kappa_5}D_y \pm iD_z)/\sqrt{2}$ with $q^2 = \sqrt{\kappa_5/\kappa_2}/H$, the gradient portion of the free energy can be written as

$$f_{grad} = \sqrt{\kappa_5\kappa_2}H\{\eta_x^*[1+2N]\eta_x + \eta_y^*[(\frac{1}{2} + \frac{1}{2\kappa_2})(1+2N) + (\frac{1}{2\kappa_2} - \frac{1}{2})(\Pi_+^2 + \Pi_-^2)]\eta_y\}.$$

Assuming that $\kappa_2 < 1$ the first transition is given by the standard hexagonal Abrikosov vortex lattice solution for η_x . To find the second transition the lowest eigenstate of $(\frac{1}{2} + \frac{1}{2\kappa_2})(1+2N) + (\frac{1}{2\kappa_2} - \frac{1}{2})(e^{2i\theta}\Pi_+^2 + e^{-2i\theta}\Pi_-^2)$ must be found (where θ has been introduced so that the vortex lattice can be rotated with respect to the ionic lattice) and a vortex lattice solution for η_y must be constructed from this. Note that the zeroes of the η_x lattice and the zeroes of the η_y lattice need not coincide [12]. This method yields for the ratio of the second transition (H_2) to the upper critical field (H_{c2})

$$\frac{H_2}{H_{c2}^{ab}} = \frac{\beta_A - \beta_m}{\beta_A \sqrt{1/\kappa_2} - \beta_m} \quad (3)$$

where $\beta_A = 1.1596$, $\beta_m = \frac{(1 - \beta_2 + \beta_3)S_1 - |\beta_2 S_2|}{|\eta_1|^2 |\eta_2|^2 / (|\eta_1|^2 |\eta_2|^2)}$, $S_1 = \frac{(\eta_1 \eta_2^*)^2}{(|\eta_1|^2 |\eta_2|^2)}$, $S_2 = \frac{(\eta_1 \eta_2^*)^2}{(|\eta_1|^2 |\eta_2|^2)}$, the over-bar denotes a spatial average, and β_m must be minimized with respect to θ and the displacement between the zeros of the η_x and the η_y lattices. Diagrams of the predicted vortex structures are shown in Fig. 1 and the phase diagram for the weak-coupling limit is shown in Fig. 2. Two vortex lattice configurations are found to be stable as a function of ν . For $-0.23 < \nu < 1$ (Phase 1), the displacement between the the zeroes of the η_x and η_y lattices is one half of a hexagonal lattice basis vector and θ varies with ν (and in general with field and temperature) so that the vortex lattice is not aligned with the ionic lattice. For $-1 < \nu < -0.23$ (phase 2), the η_x and η_y lattices coincide and a vortex lattice basis vector lies along the \hat{y} direction. Kita [11] has argued that for phase 1, at some field below H_2 there will be a first order transition from

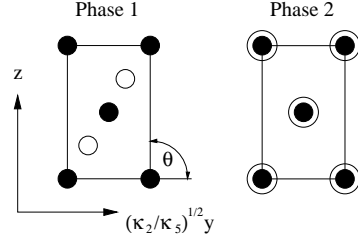


Figure 1. Stable vortex lattice structures found for the field along \hat{x} . The open (closed) circles correspond to zeroes of the η_x (η_y) lattice.

phase 1 to phase 2. For the field along $\hat{x} \pm \hat{y}$ the phase diagram is given by replacing ν with $-\nu$. Recent experiments of Mao *et al.* [13] show some support for the theory presented here.

4. Magnetic field along the c -axis

The free energy in Eq. 1 in the weak coupling limit has been used to determine the vortex lattice structure for the field along the c -axis for fields near the upper critical field [14]. The main conclusion of this analysis is that vortex lattice is square for $|\nu| > 0.0114$ and that the vortex lattice is oriented along the crystal lattice for $\nu < -0.0114$ and rotated 45 degrees from the crystal lattice for $\nu > 0.0114$. The analysis near H_{c1} has also been carried out with the result that the vortex lattice at H_{c1} will be hexagonal and with increasing field the lattice will continuously distort until a square vortex lattice is formed [15]. A square vortex lattice has been observed by Small Angle Neutron scattering (SANS) and the orientation implies $\nu > 0.0114$ [8]. One notable feature of the SANS measurements is the observation of Bragg peaks beyond the first Bragg peak. The analysis of Eq. 1 has been extended to fields below H_{c2} and the lowest Bragg peaks of the field distribution have been calculated and compared to experiment. One comparison is shown in Fig. 3 (note that in the SANS measurements there is flux pinning which is not included in the calculations). The large size of the higher order Bragg peaks relative to that expected for a single

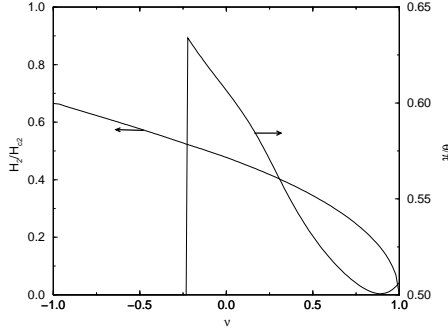


Figure 2. The ratio of the two transition fields and θ (the angle relating the orientation of the vortex lattice to the ionic lattice) as a function of ν .

complex order parameter component (Abrikosov) theory and the agreement between the theory and the experiment gives support to the E_u theory. However, note that it is possible that an Abrikosov theory with sufficiently large non-local corrections may also account for the observed results.

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REFERENCES

1. Y. Maeno *et al.*, Nature **372**, 532 (1994).
2. K. Ishida *et al.*, Phys. Rev. B **56**, 505 (1997).
3. A.P. Mackenzie *et al.*, Phys. Rev. Lett. **80**, 161 (1998).
4. K. Ishida *et al.*, Nature (London) **96**, 658 (1998).
5. T.M. Rice and M. Sigrist, J. Phys.: Condens. Matter **7**, L643 (1995).

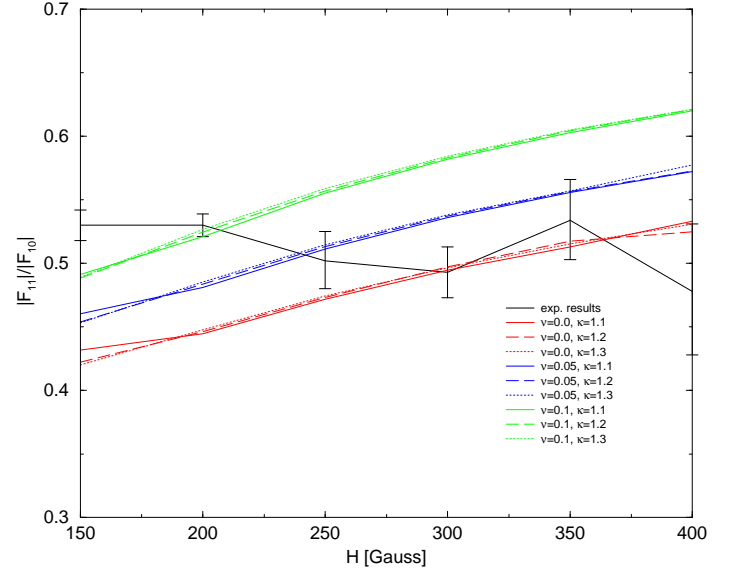


Figure 3. Comparison between the weak-coupling E_u theory and experimental results for the ratio of the spatial Fourier components of the field corresponding to the (1, 0) and (1, 1) Bragg peaks of the square vortex lattice.

6. M. Sigrist and K. Ueda, Rev. Mod. Phys. **63**, 239 (1991).
7. G.M. Luke *et al.*, Nature **394**, 558 (1998).
8. T.M. Riseman *et al.*, Nature **396**, 242 (1998); and correction in press (2000).
9. D.F. Agterberg, Phys. Rev. Lett. **80**, 5184 (1998).
10. I.A. Luk'yanchuk and M.E. Zhitomirsky, Supercond. Rev. **1**, 207 (1995).
11. T. Kita, Phys. Rev. Lett. **83**, 1846 (1999).
12. R. Joynt, Europhys. Lett. **16**, 289 (1991); A. Garg and D.C. Chen, Phys. Rev. B **49**, 479 (1994).
13. Z.Q. Mao *et al.*, Phys. Rev. Lett. **84**, 991 (2000).
14. D.F. Agterberg, Phys. Rev. B **58**, 14 484 (1998).
15. R. Heeb and D.F. Agterberg, Phys. Rev. B **59**, 7076 (1999).